Machine Learning for Neuroscience

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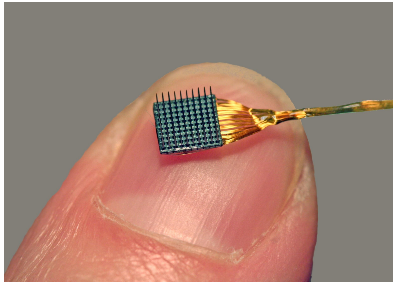
Some figures derived from slides by Tom Mitchell, Aarti Singh, Ziv Bar-Joseph, and Alona Fyshe

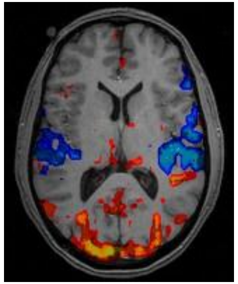
Goal: intuitive understanding of ML methods and how to use them

- we'll use scikit-learn: http://scikit-learn.org/stable/
- brief homeworks after each class, both critical thinking and using scikit-learn
- video tape each lecture and put videos on Youtube after each class

How can ML help neuroscientists?

- ❏ Deal with large number of sensors/recording sites





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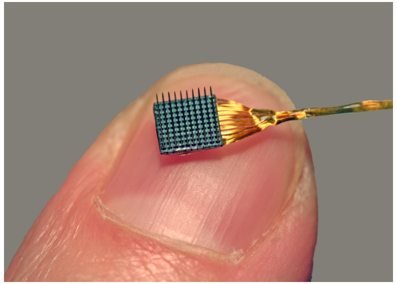

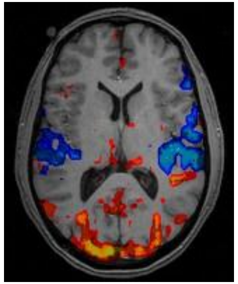

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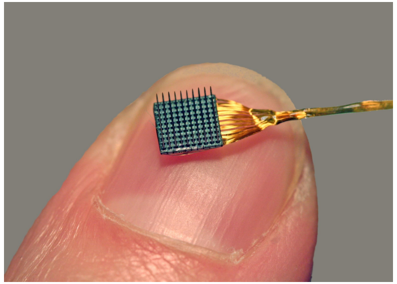

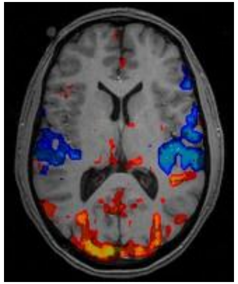

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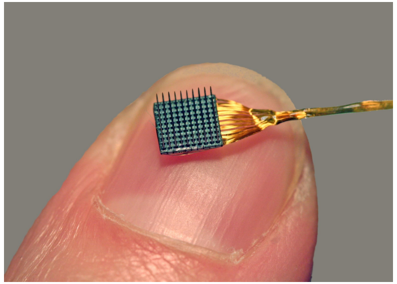

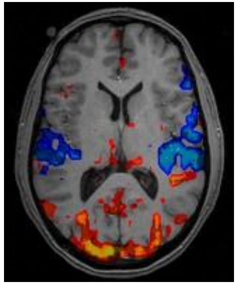

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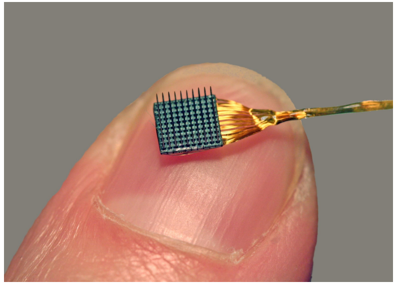

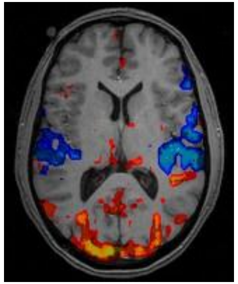

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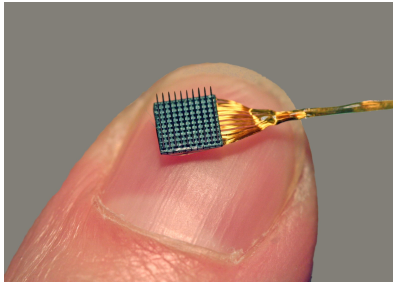

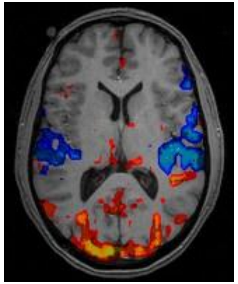

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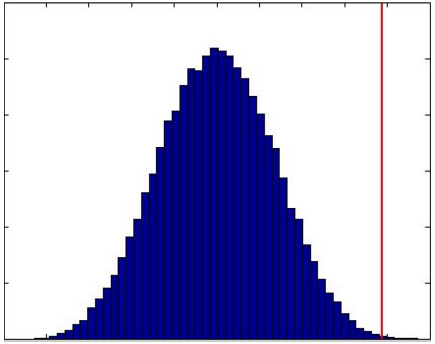

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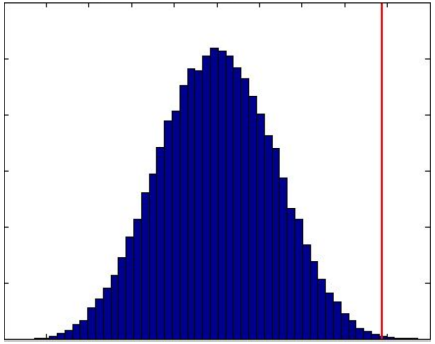

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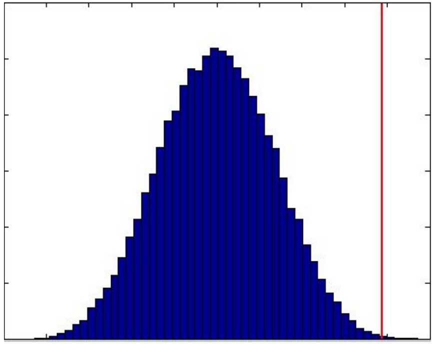

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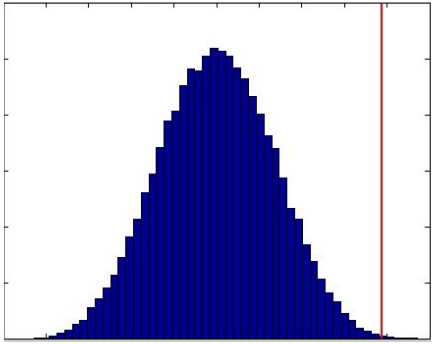

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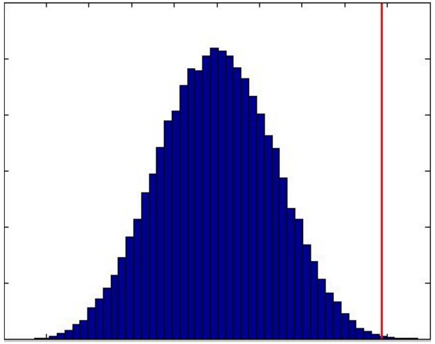

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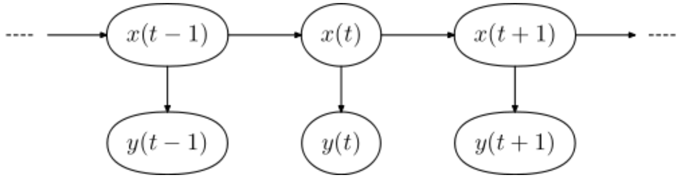
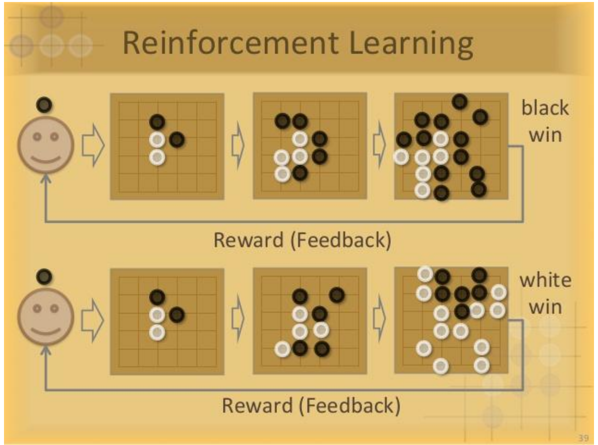
- Complex data-driven hypotheses of brain processing
  - advanced topics: latent variable models, reinforcement learning, deep learning





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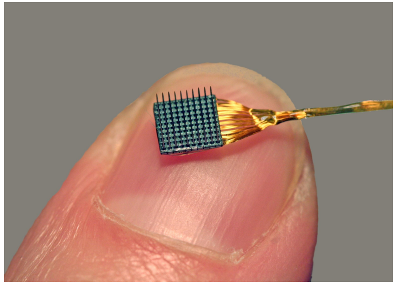

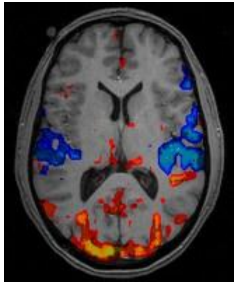

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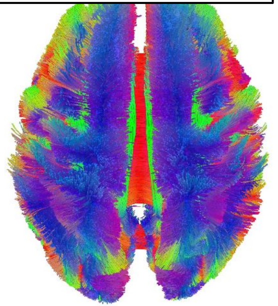
Today: classification and regression

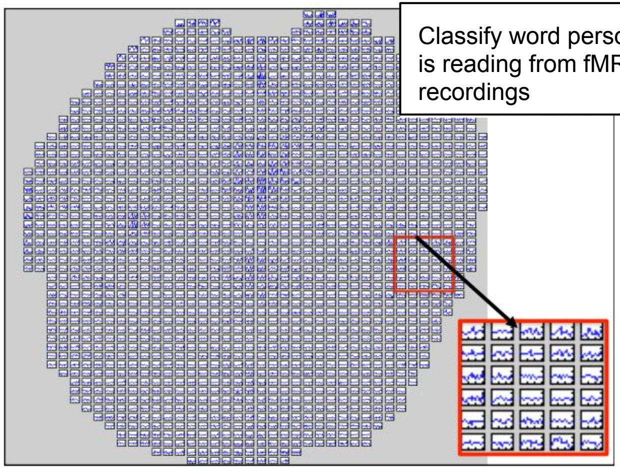
- Classification methods:
  - naive Bayes
  - support vector machine (SVM)
  - k-nearest-neighbors (kNN)
- Regression:
  - linear

Classification: example problems

Classify DTI fiber tracks into anatomical bundles



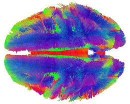
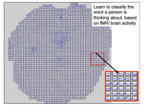
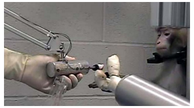
Classify word person is reading from fMRI recordings



Classify direction of desired movement from motor cortex recordings

What is a classifier?

- ❑ Any algorithm that can assign a class label to each data instance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	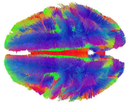	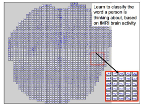	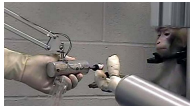
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	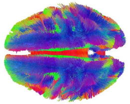	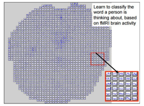	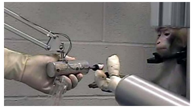
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	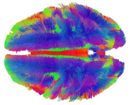	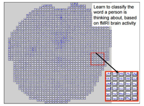	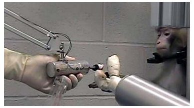
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	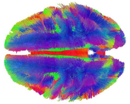	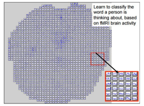	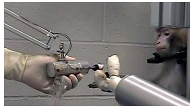
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	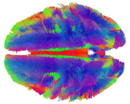	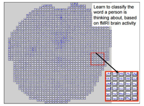	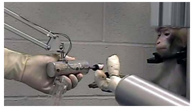
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	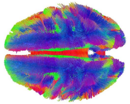	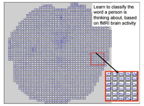	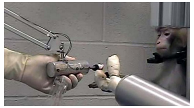
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	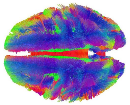	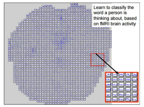	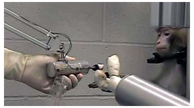
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- Input: feature vector for each data instance
- Output: class label

Classifiers divide in roughly 3 types

- Generative
  - Build a generative statistical model
    - Naive Bayes
- Discriminative
  - Directly estimate a decision rule or boundary
    - SVM
- Instance based classifiers
  - Use observations directly without building a model
    - kNN

How do most classifiers work? 3 main steps!

Assume: Make an assumption about the data

- e.g. assume all values of voxels recorded during the presentation of the same word follow a Gaussian distribution

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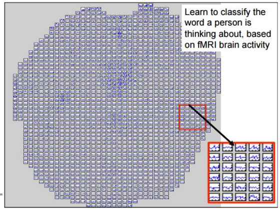
Test: Apply learned model to new data

- e.g. using the learned mean and covariance for each word class, calculate how likely it is for a new data instance to belong to each class

Problem with train step: too many parameters to estimate can lead to their inaccurate estimation



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Let us be interested in a region of interest with 30 voxels
Let the person only read 2 words: “chair” and “celery”

v_1	v_2	...	v_{29}	v_{30}	w
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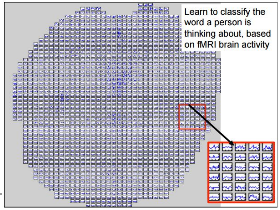

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- Parameter = P(w = “chair”|v_1=0,v_2=1,...v_{29}=1,v_{30}=0) => ~2^{30} parameters
- Need more instances than parameters to estimate correctly => lots of data!

Reduce number of parameters using Bayes rule

$$\mathbb{P}(w|v_1, v_2, \dots v_{29}, v_{30}) = \frac{\mathbb{P}(v_1, v_2, \dots v_{29}, v_{30}|w)\mathbb{P}(w)}{\mathbb{P}(v_1, v_2, \dots v_{29}, v_{30})}$$

- How many parameters for $P(v_1,v_2,...v_{29},v_{30}|w)$? $\sim 2^{30} x2$!

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$$\mathbb{P}(v_1, v_2, \ldots v_{29}, v_{30}|w) = \prod_{i=1}^{30} \mathbb{P}(v_i|w)$$

- ❑ Now, how many parameters for $P(v_1,v_2,...v_{29},v_{30}|w)$? 2x30 = 60
- ❑ Huge reduction of parameters, but a very strong assumption

What about when features aren't discrete? Gaussian Naive Bayes

v_1	v_2	...	v_{29}	v_{30}	w
0.22	0.80	...	0.89	0.20	"chair"
0.14	0.31	...	0.23	0.45	"celery"
0.53	0.67	...	0.01	0.43	"celery"

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$$\mathbb{P}(v_i = 0.22 | w = chair) = \frac{1}{\sqrt{2\pi\sigma_{i,chair}^2}} e^{\frac{1}{2}\left(\frac{0.22-\mu_{i,chair}}{\sigma_{i,chair}}\right)^2}$$

Gaussian Naive Bayes: estimation of parameters

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- Want to estimate $\mu_{i,chair}$, $\sigma_{i,chair}$, $\mu_{i,celery}$, $\sigma_{i,celery}$ for all i
- $\mu_{1,chair}$ = average the values of v_1 during all presentations of "chair"
- $\sigma_{1,chair}$= find standard deviation of the values of v_1 during all presentations of "chair"

Gaussian Naive Bayes: testing

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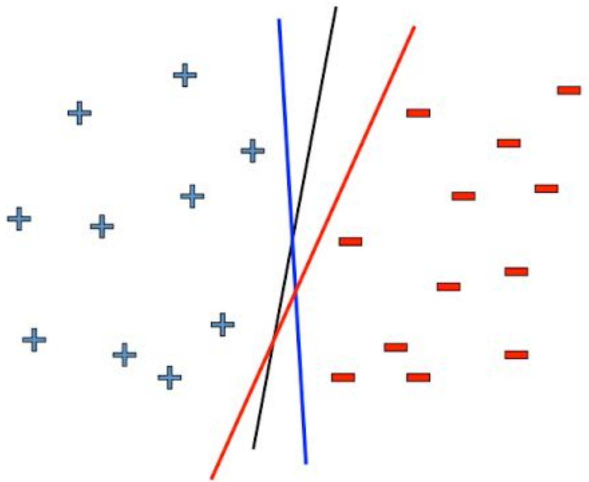
- Assign the class with higher probability to the new data instance

Naive Bayes takeaways

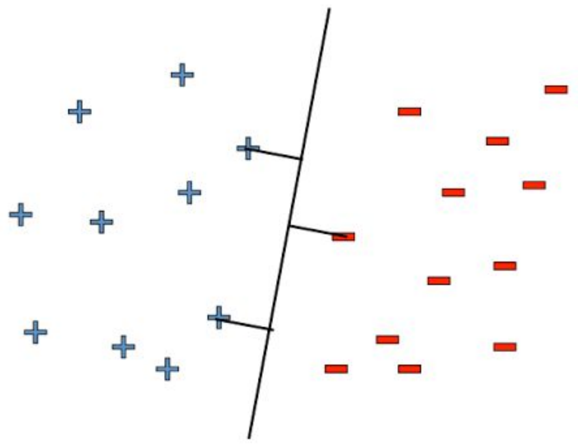
- Reduced number of parameters to estimate
- Fast training
- Can be used to quickly classify very high-dimensional data instances
- But makes strong conditional independence assumption

Support Vector Machines (SVM): motivation

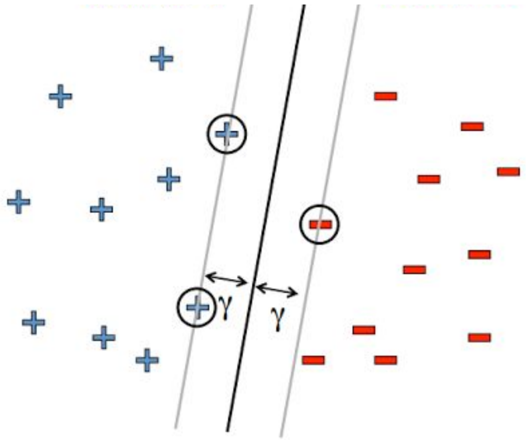
Want to directly learn a classification boundary, but which boundary is better?



SVM: choosing a decision boundary with the largest margin

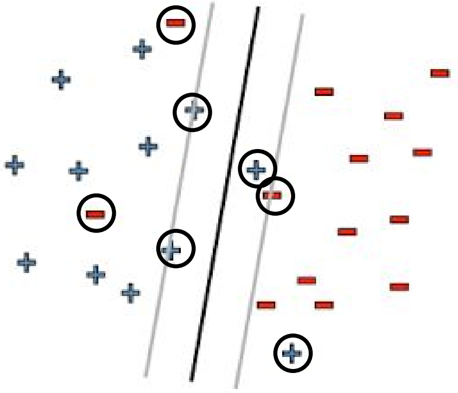


What are support vectors?



- Data points that are a margin-width away from the decision boundary
- Only need to store the support vectors to predict labels for new points => efficiency

What if data isn't linearly separable? Allow error in classification => soft-margin SVM



- Trade-off between maximizing the margin and minimizing the number of mistakes on the training data

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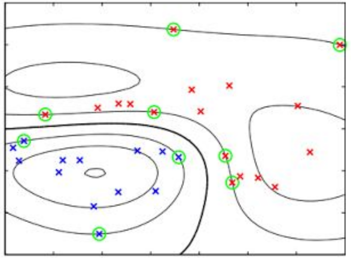
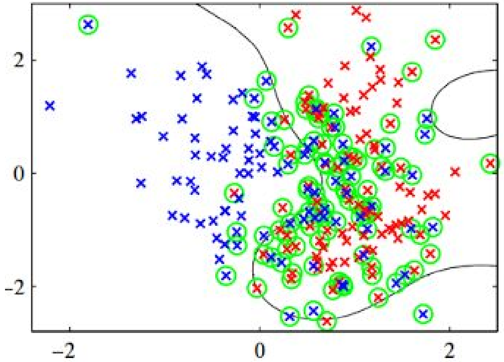
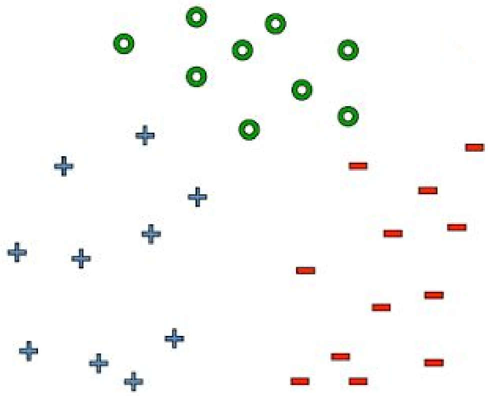
  - One common kernel is the Gaussian kernel (RBF):



$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||^2}{2\sigma^2}\right)$$



What if we have multiple classes? Multi-class SVM



- Margin = gap between correct class and nearest other class

SVM takeaways

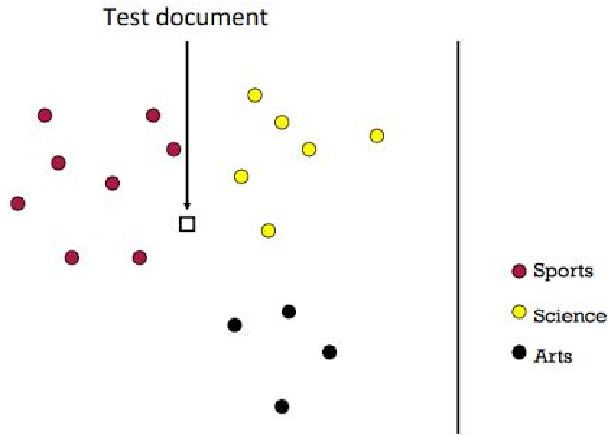
- Directly estimates the decision boundary
- Space-efficient
- Can handle non-linearly separable data through various kernel functions
- Does not directly output probabilities for classifications

k-Nearest Neighbors classifier: even fewer assumptions!

- Does not assume a model = non-parametric method
  - Number of parameters scale with the number of training data
  - Free from strong distributional assumptions that are not satisfied in practice
  - But needs lot of data to learn complex models

kNN: an intuitive algorithm

- We wish to classify a test instance



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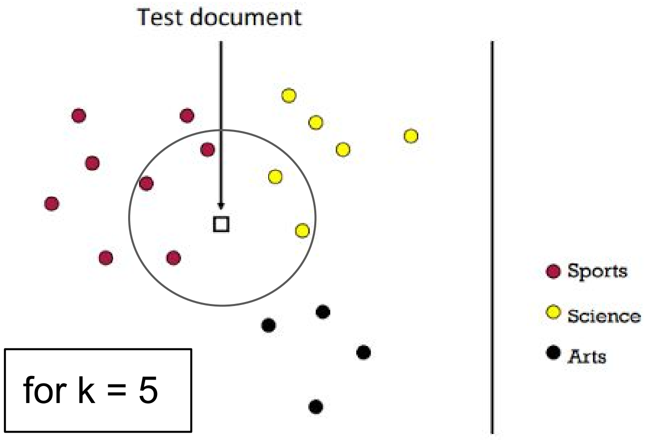
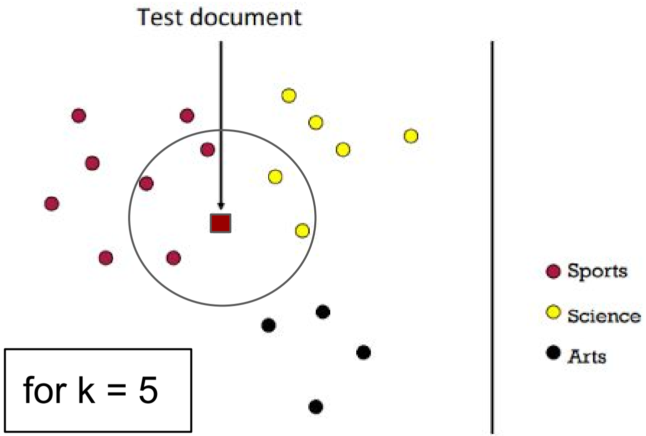


kNN: an intuitive algorithm

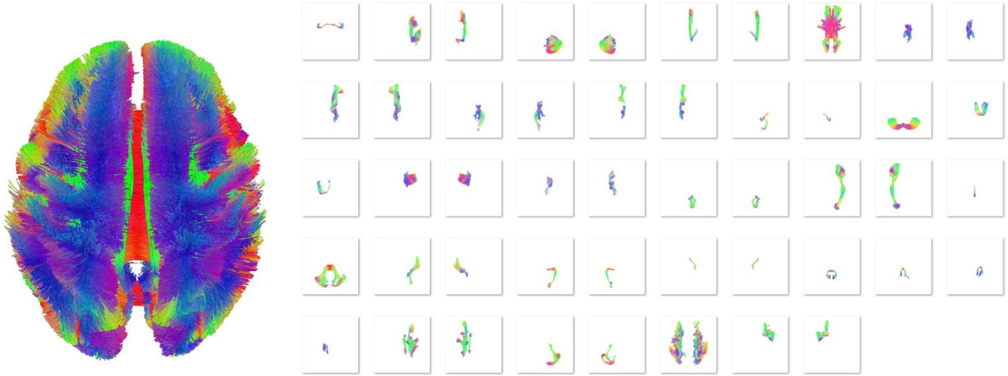
- We wish to classify a test instance
- Find the k closest training data instances to the test instance
- Assign test instance with label of the majority within the k closest instances



How to choose k?

- Trade-off between stability and accuracy
  - Larger k is more stable
  - Smaller k is more accurate
- Depends on type and amount of training data

kNN in practice: classifying DTI fibers into bundles



kNN takeaways:

- Requires a lot of data
- Requires storage and computation on entire data set
- Powerful classification technique if enough data available, and if there are no problems with data storage

Classification vs regression

- Classification = output is class label (“chair”, “celery”)
  - classify the word a subject was reading from fMRI voxels

- Regression = output is continuous value (<0.2, 0.3,...,0.9>,<0.7,0.3,...,0.1>)
  - predict next fMRI voxel values from previous voxel values

Regression: general

- Choose a parametric form for P(labels|data;θ)
- Derive a learning algorithm to estimate parameters θ

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- To solve, take derivative and set equal to 0. Closed-form solution available for simple f(x), otherwise use gradient descent

Takeaways

- 3 types of classifiers
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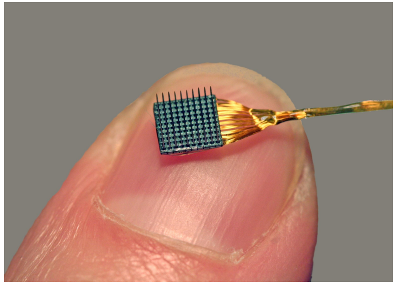
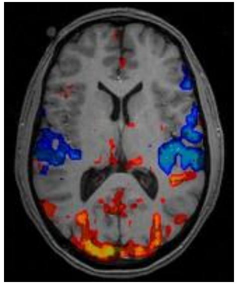
- Regression can be used to predict continuous values

Next time: model selection & dimensionality reduction

- Deal with large number of sensors/recording sites





- investigate high-dimensional representations
  - classification (what does this high-dimensional data represent?)
  - regression (how does it represent it? can we predict a different representation?)
  - **model selection (what model would best describe this high dimensional data?)**
- **uncover few underlying processes that interact in complex ways**
  - **dimensionality reduction techniques**